UCRL- 99731
PREPRINT

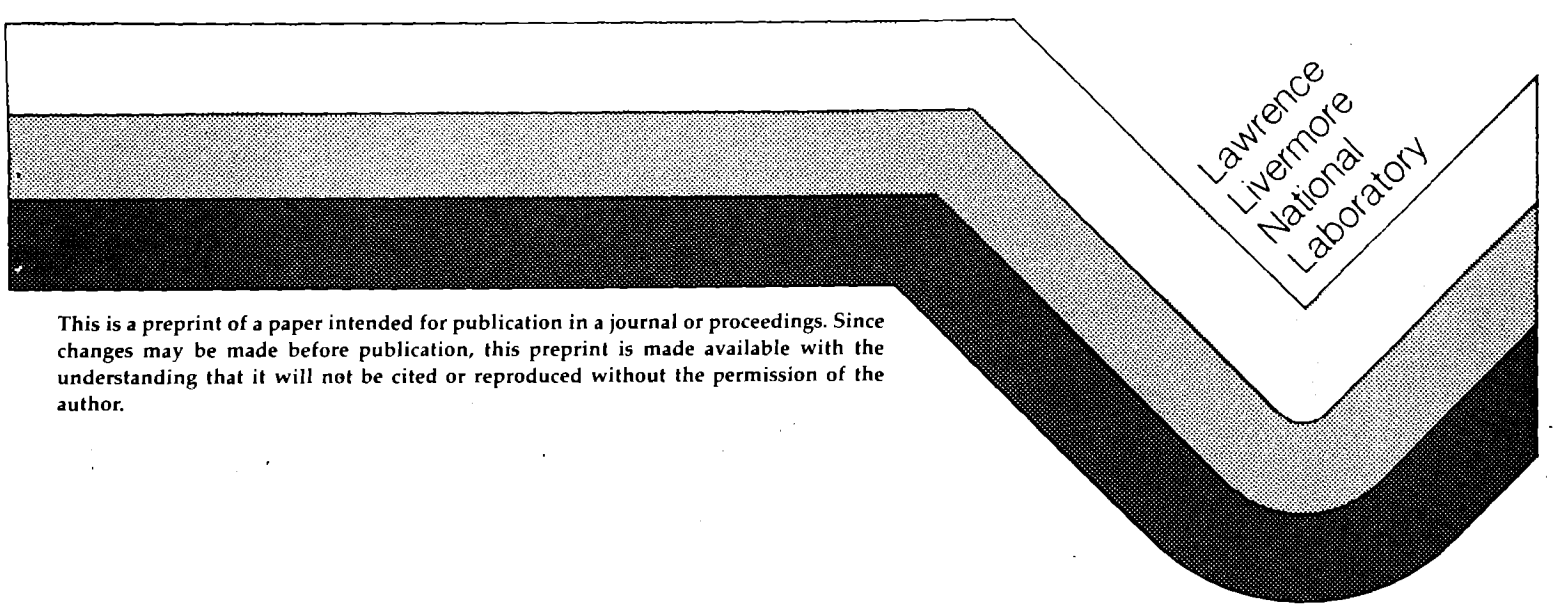
DPDC: A SECOND-ORDER MONOTONE SCHEME FOR ADVECTION

C. W. Beason

L. G. Margolin

This paper was prepared for submittal to
Fifth Nuclear Code Developers' Conference
October 11-14, 1988, Boulder, CO

September 26, 1988



DPDC: A SECOND-ORDER MONOTONE SCHEME FOR ADVECTION

C. W. Beason†
L. G. Margolin
Lawrence Livermore National Laboratory
Livermore, CA

ABSTRACT

We are developing a new, second-order, monotone scheme for advection. DPDC (i.e., double-pass donor cell) is based on Smolarkiewicz' simple, positive definite method. Both schemes are multipass methods in which upstream approximations to the truncation error are subtracted from the equations. We describe two significant improvements to Smolarkiewicz' method. First, we use a local gauge transformation to convert the method from being positive definite to the stronger condition of being monotone. Second, we analytically approximate the sum of the corrections of all the passes to use in a single corrective pass. This increases the accuracy of the method, but does not increase the order of accuracy. We compare DPDC with van Leer's method for advection of several different pulses in a constant velocity field.

INTRODUCTION

The solution of the advection equation is a necessary feature of continuous rezone (ALE) codes[1] that simulate fluid flow. The advection algorithm must be accurate in the sense of adding little numerical diffusion to the solution. Also the algorithm must be stable and reasonably free of nonphysical oscillations. Donor cell, which is sometimes called upstream differencing, is nearly monotone. However, donor cell has only first order accuracy, and leads to excessive numerical smoothing of the solution in regions of steep gradients. On the other hand, higher-order methods such as interpolated donor cell[1] can develop large oscillations in those same regions of steep gradients. Centered differencing is unconditionally unstable.

A new class of schemes that are second-order accurate and monotone have been evolving over the past 15 years. Some of these schemes are based on flux-limiting.[2] Here a high-order method is used to calculate fluxes and to construct a trial solution. This trial solution is then examined for new maxima and minima that can be identified as being nonphysical. In regions where these new nonphysical structures are present,

---

† Captain, United States Air Force, currently assigned to Lawrence Livermore National Laboratory.

one blends in sufficient amounts of a low-order flux to preserve monotonicity. An alternate approach[3] is to attempt a higher-order reconstruction of the discrete field to be advected. (Donor cell is equivalent to a piecewise constant reconstruction.) In these schemes it is the variation of the reconstructed function that is limited. Both of these approaches are similar in being based on preserving monotonicity of the solution.

Smolarkiewicz' simple positive definite scheme[4,5] is not based on preserving monotonicity, but rather on the desirable properties of upstream differencing itself. The basic idea is simple. Smolarkiewicz notes that the lowest order truncation error associated with using donor cell advection is proportional to the second spatial derivative of the field, and so the effective equation that we solve numerically is an advection-diffusion equation. He formally rewrites the diffusion term in the form of an advection term, where the velocity field (termed pseudo velocities) is based on the truncation error and is independent of any physical velocity. Then he approximates this new advection term, again using donor cell, and subtracts it. Since this is a first order approximation to a second order term, the error is third order, meaning that the overall scheme formally has second order accuracy. Note that this error can itself be approximated in the same manner, and subtracted. This further reduces the magnitude of the truncation error, but does not affect its order. (Increasing the order of the scheme would require introducing more points into the difference stencil.)

Smolarkiewicz proposed his scheme as a simple and computationally cheaper alternative to the monotonicity preserving methods. However, we believe that it has other advantages for multidimensional flows, especially on irregular meshes. These advantages are associated with the scheme being naturally unsplit in space. The scheme as published also has a few disadvantages. These are mainly associated with the fact that it is positive definite, but not monotonic. Advected fields may exhibit small oscillations in the neighborhood of steep gradients. The scheme also does not preserve the maximum value of sharp peaks, and in general allows more numerical diffusion than the mono-tonicity preserving schemes.

In DPDC (double-pass donor cell) we have created an advection scheme that is monotone and accurate while preserving the simplicity and the unsplit nature of Smolarkiewicz' basic method. The purpose of this paper is to describe two of these improvements. In the next section we will briefly review Smolarkiewicz' method. Then we will describe the use of local gauge transformations to convert the positive definite algorithm into a monotone algorithm. We will next show how to approximately sum the estimates of the truncation to all orders as a perturbation series in the Courant number.

Finally we will show calculations of advection of several different pulses, comparing our new method with Van Leer's method.[3]

SIMPLE POSITIVE DEFINITE ADVECTION SCHEME

Consider the one-dimensional mesh shown in Fig. 1 with uniform cell size.

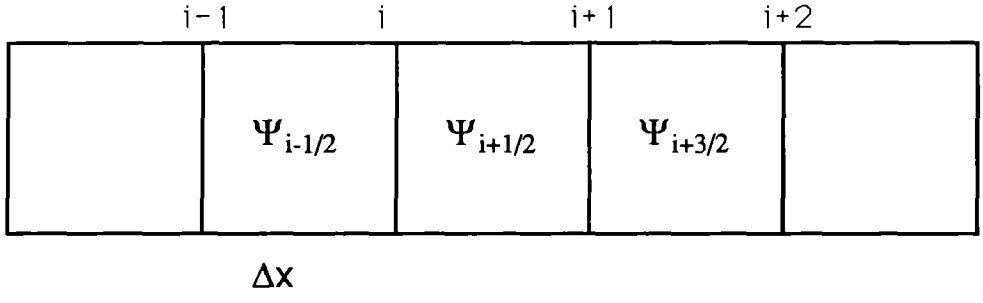


Figure 1. A one-dimensional mesh with uniform cell size. The nodes are labeled by the index i. The field to be advected is stored at the cell centers and labeled by half integers.

The donor cell, or upstream advection scheme is defined by

$$(1) \qquad \Psi^{N+1}_{i+1/2} = \Psi^{N}_{i+1/2} - F\left(\Psi^{N}_{i+1/2}, \Psi^{N}_{i+3/2}, u^{N}_{i+1}\right) + F\left(\Psi^{N}_{i-1/2}, \Psi^{N}_{i+1/2}, u^{N}_{i}\right)$$

where F is the flux function

$$(2) \qquad F\left(\Psi_{i-1/2}, \Psi_{i+1/2}, u\right) = \left[\Psi_{i-1/2}(u + |u|) + \Psi_{i+1/2}(u - |u|)\right] \frac{\Delta t}{2\,\Delta x}$$

Here $\Psi^{N}_{i-1/2}$ is the value of Ψ at the cell center i-1/2, and at the N^{th} time step. The time step is Δt and the width of a cell is Δx. The donor cell scheme in Eq. (1) is positive definite if the Courant number is less than 1. (The scheme is monotone if the velocity field u is spatially constant.) Expanding Eq. (1) in a Taylor series to second order

$$(3) \qquad \frac{\partial \Psi}{\partial t} = -\frac{\partial (u\Psi)}{\partial x} + \frac{\partial}{\partial x}\left[\frac{(|u|\Delta x - u^2 \Delta t)}{2} \frac{\partial \Psi}{\partial x}\right]$$

From Eq. (3) we see that the donor cell scheme approximates not the advection equation, but an advection-diffusion equation. The trick now is to express the diffusion term as an advection term. We define an antidiffusive velocity v by

$$(4) \qquad v^{(1)} = \left[\frac{(|u|\Delta x - u^2 \Delta t)}{2\Psi} \frac{\partial \Psi}{\partial x} \right]$$

Now we can reverse the effects of the diffusion term by adding the antidiffusive velocity to the advection velocity in the donor cell step. This is equivalent to subtracting a donor cell estimate of the truncation error at every point.

We have denoted the antidiffusive velocity with the superscipt (1). (N.B. superscripts are always shown inside parentheses to distinguish them from exponents.) After subtraction, the new equation can be Taylor-expanded and shown to be

$$(5) \qquad \frac{\partial \Psi}{\partial t} = -\frac{\partial (u\Psi)}{\partial x} + \frac{\partial}{\partial x}\left[\frac{(|v^{(1)}|\Delta x - [v^{(1)}]^2 \Delta t)}{2} \frac{\partial \Psi}{\partial x} \right]$$

This means that we could repeat the process defining another antidiffusive velocity $v^{(2)}$ in terms of $v^{(1)}$. This process can be repeated indefinitely; the magnitude of the error will be reduced after each extra step.

An important point here is that the values of Ψ used numerically to evaluate the antidiffusive velocities are those that enter the cycle -- i.e., at time N -- and not those after a first donor cell pass using only the velocity field u as suggested in Smolarkiewicz' paper. That is, the scheme does not have to be multipass. There are advantages to using a two-pass system, but in either case for better accuracy, the antidiffusive velocities should all be evaluated using N-time information. In fact, for reasons that we will describe later, we prefer to use a two-pass formalism.

MONOTONICITY

Monotone schemes and positive schemes are closely related. To begin, we note that the advection equation with a spatially varying velocity field is not invariant under a simple change of the zero point of the field --i.e., under a gauge transformation. Now consider the transport of a square wave pulse through a background that is constant and nonzero. After several cycles using the positive definite scheme, small oscillations will develop around the leading and trailing edges of the pulse. These oscillations are

a purely numerical effect, since the solutions to the continuum equation are monotone. Now if the background were at a zero level, then these oscillations would vanish. The valleys are eliminated by the positive definite property of the algorithm. The peaks must also vanish; because of conservation, they can only occur in conjunction with the valleys. Thus, if we have any pulse being transported through a constant background of level Ψ^m , we can convert a positive definite scheme into a monotone scheme by

1. global scaling of the field so that the background vanishes;
2. advecting the scaled field, and
3. rescaling the advected field to its original zero point.

Global scaling is simple, but is not useful in most circumstances. A more powerful idea is a local rescaling in which the gauge varies at every interface. The local zero point at an interface is chosen as the minimum value of the field in the two neighboring cells and in each of the nearest neighbors of those cells. In the one-dimensional example, the local minimum at the interface i is

$$(6) \qquad \Psi_i^{min} = \min \{\Psi_{i-3/2}, \Psi_{i-1/2}, \Psi_{i+1/2}, \Psi_{i+3/2}\}$$

The gauge transformation is closely related to the concept of flux-limiting in schemes like FRAM and FLOE.[2]

A similar technique can be applied to local maxima. In this case one transforms the maxima into minima by reflecting the entire field -- i.e., by multiplying by (-1). Then one follows the same recipe outlined above for minima. The choice of the local maximum gauge is also similar to Eq. (6) with the max function replacing the min function.

For general pulses, the remaining question is when to use the minimum gauge and when to use the maximum gauge. The answer (for reasons that we will not explain here) depends on the sign of the second spatial derivative. When the function is concave (the second derivative is positive), one uses the minimum gauge and when the function is convex, one uses the maximum gauge. Note that when the function is linear and the second derivative vanishes, the two gauges are equivalent assuring a smooth transition.

There are several points that are worth mentioning in connection with the local gauge transformation. First, using the gauge transformation means that the actual zero point of the field becomes irrelevant. Thus, the fields we transport no longer need to be positive definite. This is useful for dealing with the fluid equations, for the momenta may be either positive or negative.

Second, the principal effect of the gauge transformation lies in altering the magnitude of the antidiffusive velocity defined in Eq. (4). Consider a region in which the field is exactly linear. In the positive definite scheme, the antidiffusive velocity will depend inversely on the magnitude of Ψ and so will vary in space. After advection, the profile will no longer be linear even if the advection velocity u is constant in space. After the local gauge transformation, the antidiffusive velocity will depend inversely on $(\Psi - \Psi^m)$, and in a linear profile will be constant. Thus, using the local gauge allows us to preserve the slope in regions of linear variation. We note that the monotonicity preserving schemes tend to oversteepen gradients and in general do not preserve slopes.

Finally, let us return to the point of deciding between the minimum and the maximum gauge. We noted that this decision is based on the sign of the second derivative at the interface. Computationally, the natural centering for the second derivative is at the cell center, not the interface. This inconvenience can be avoided by using the advection equation to convert one spatial derivative into a time derivative. Thus, our decision is made by comparing the first spatial derivative across the interface before and after a regular donor cell step. The sign of this difference, multiplied by the sign of the velocity field, is the sign of the second spatial derivative. Furthermore, this concept generalizes easily to two dimensions. It also can be applied to more general meshes of cells that are not quadrilaterals, for example, for free Lagrange calculations.

SUMMING THE SERIES

Equation (4) defines a recursive relation for the antidiffusive velocity $v^{(k)}$ that estimates the error of the k^{th} pass. We can rewrite this relation is dimensionless form

$$(7) \quad V^{(k)} = A\left(\left|V^{(k-1)}\right| - \left[V^{(k-1)}\right]^2\right) \quad \text{where } A \equiv \frac{\Delta x}{\Psi}\frac{\partial \Psi}{\partial x};\ V^{(k)} = \frac{v^{(k)}\Delta t}{\Delta x}$$

and the spatial index is suppressed. The first term, $V^{(1)}$ is defined by Eq. (4). We again note that A is a constant evaluated from the field values at the beginning of the cycle, and does not change. Using a large number of passes, each with its own antidiffusive velocity, to reduce the error is equivalent to doing a single pass with the sum of all the velocities

$$(8) \quad W = \sum_{k=1}^{\infty} V^k$$

The chief result of this section is that we can perform this sum approximately in the sense of a perturbation series where the small variable is the dimensionless quantity $V^{(1)}$. It is possible to show that

$$(9) \quad \left| \frac{u\,\delta t}{\delta x} \right| \le 1 \text{ and } |A| \le 1 \Rightarrow \left| V^{(1)} \right| \le 1$$

The first condition is guaranteed by the Courant condition, and the second condition is a result of the gauge transformation.

We expand each term of the recursion in powers of $V^{(1)}$.

$$(10) \quad V^{(k)} = \alpha^{(k)} V^{(1)} + \beta^{(k)} [V^{(1)}]^2 + \gamma^{(k)} [V^{(1)}]^3 + \delta^{(k)} [V^{(1)}]^4 + \ldots$$

Next, substitute this expansion into the recursion Eq. (7). The absolute value inside the recursion requires us to distinguish between two cases. If A is positive, then V^k is positive for all values of k. Alternately, if A is negative, then V^k is also negative for all values of k. Let us assume that A is positive. Then

$$(11) \quad \begin{aligned} V^{(k+1)} &= A[V^{(1)}]\{\alpha^{(k)}\} + A[V^{(1)}]^2 \{\beta^{(k)} - \alpha^{(k)}\alpha^{(k)}\} \\ &\quad + A[V^{(1)}]^3 \{\gamma^{(k)} - 2\alpha^{(k)}\beta^{(k)}\} + \ldots \end{aligned}$$

Since there is a series expansion for $V^{(k+1)}$ like Eq. (10) , we have the set of recursive relations for the various subseries

$$(12) \quad \begin{aligned} \alpha^{(k+1)} &= A\,\alpha^{(k)} \\ \beta^{(k+1)} &= A\{\beta^{(k)} - \alpha^{(k)}\alpha^{(k)}\} \\ \gamma^{(k+1)} &= A\{\gamma^{(k)} - 2\alpha^{(k)}\beta^{(k)}\} \\ \delta^{(k+1)} &= A\{\delta^{(k)} - 2\alpha^{(k)}\gamma^{(k)} - \beta^{(k)}\beta^{(k)}\} \end{aligned}$$

plus the initial conditions

$$(13) \quad \alpha^{(1)} = 1; \quad \beta^{(1)} = 0; \quad \gamma^{(1)} = 0; \quad \delta^{(1)} = 0; \ldots$$

Now sum the first relation of Eq. (12) over k=1,2,3, . . .

$$(14)\quad \Sigma_\alpha = \alpha^{(1)} + A\Sigma_\alpha \qquad \text{or} \qquad \Sigma_\alpha \equiv \sum_{k=1}^{\infty} \alpha^{(k)} = \frac{1}{1-A}$$

Next, sum the second relation of Eq. (12) over k=1,2,3, . . .

$$(15)\quad \Sigma_\beta = A\,\Sigma_\beta - A\,\Sigma_{\alpha\alpha} \qquad \text{where} \qquad \Sigma_{\alpha\alpha} \equiv \sum_{k=1}^{\infty} \alpha^{(k)}\alpha^{(k)}$$

To evaluate the second term of the right hand side, we multiply the recursive relation for α by itself and then sum.

$$(16)\quad \Sigma_{\alpha\alpha} = 1 + A^2\Sigma_{\alpha\alpha} \quad \text{or} \quad \Sigma_{\alpha\alpha} = \frac{1}{1-A^2}$$

Finally then

$$(17)\quad \Sigma_\beta = \frac{-A}{(1-A)(1-A^2)}$$

In general, each of the sums can be handled in this way, being reduced ultimately to the sum over some power of the $\alpha^{(k)}$ series. Also, the entire process can be repeated for the case of A being negative. The results for the first few terms, valid for A of any sign are

$$\Sigma_\alpha = \frac{1}{1-|A|} \qquad \Sigma_\beta = \frac{-A}{(1-|A|)(1-A^2)}$$

(18)

$$\Sigma_\gamma = \frac{2A^3}{(1-|A|)(1-A^2)(1-|A|^3)}$$

Inserting these results into Eq. (8) leads to our final result

$$(19)\quad W = \Sigma_\alpha V^{(1)} + \Sigma_\beta [V^{(1)}]^2 + \Sigma_\gamma [V^{(1)}]^3 + \ldots$$

Since DPDC could be written as a single pass scheme, we must enforce a Courant like condition that the sum $|u + W| < 1$. This is a kind of flux-limiting also, but is completely local and does not require any reconstruction of the field.

RESULTS

We finish by showing some sample results of advecting several different pulses. In each case, we solve the one-dimensional advection equation with a constant velocity field in a uniform mesh. The Courant number was chosen to be 0.5. This turns out to be a special choice in that the next order of truncation error, proportional to the third spatial derivative of the field, exactly vanishes. On each figure we also plot the equivalent result using Van Leer's method.[3] In Fig. (2) we show a square wave, illustrating that we can preserve the initial maximum value and have a monotone scheme. In Fig. (3) we show a triangular wave, illustrating how well we can preserve the maximum value of a sharp pulse. In Fig. (4) we show a sine wave, illustrating that we can treat fields that are not positive definite. In each case, our method appears to as good or better than the Van Leer method.

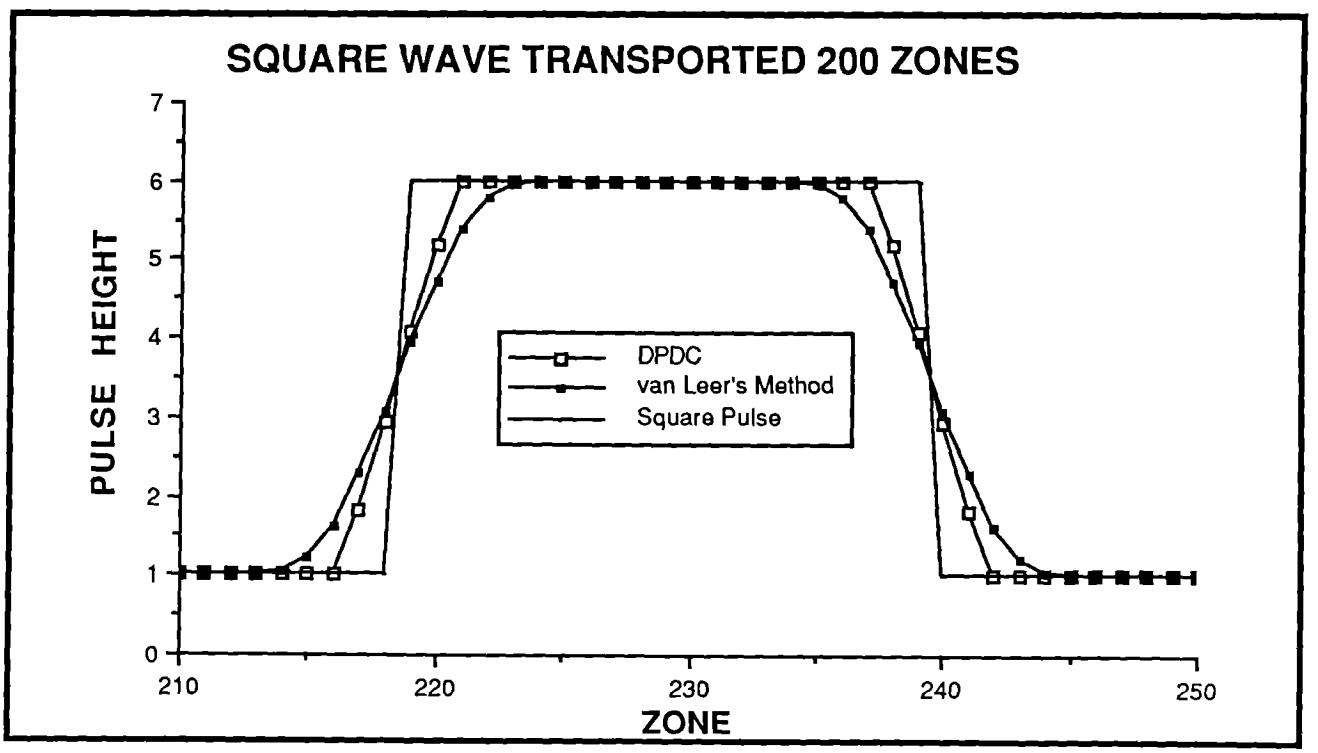


Figure 2. A simple square wave is advected with a constant velocity for 200 zones. The DPDC calculation is compared with a Van Leer scheme, and with the original profile.

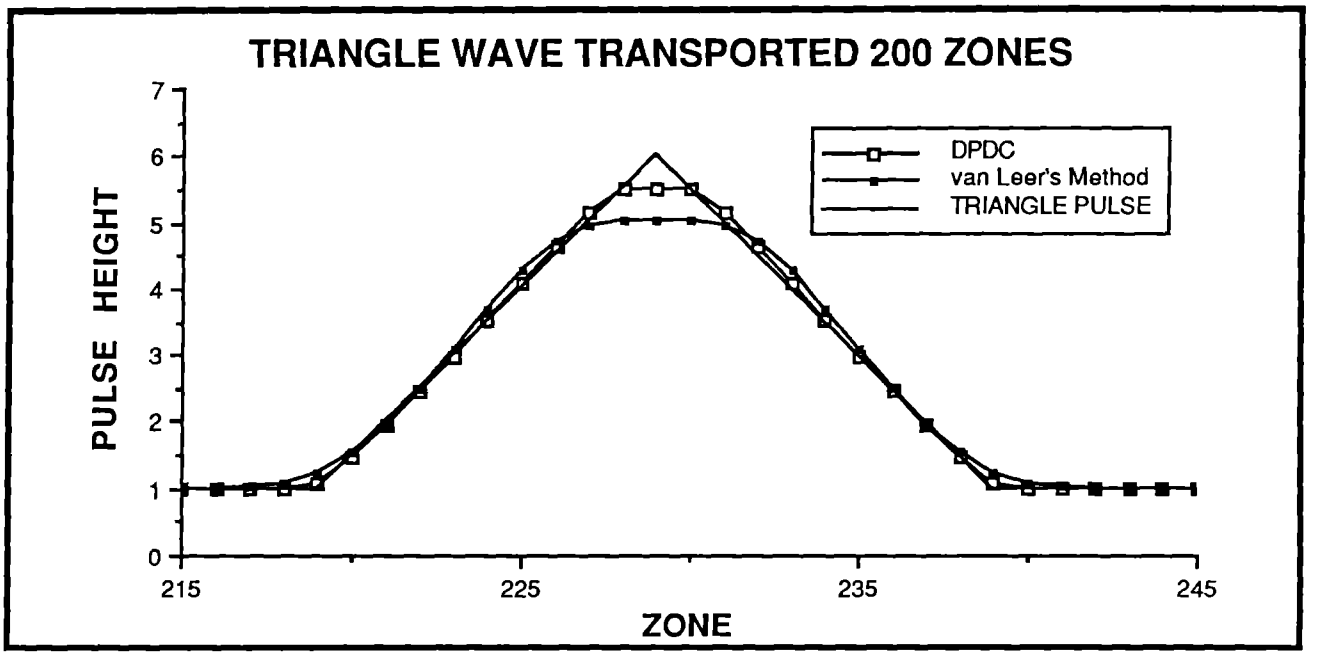


Figure 3. A triangular wave is advected with a constant velocity for 200 zones. The DPDC calculation is compared with a Van Leer scheme, and with the original profile.

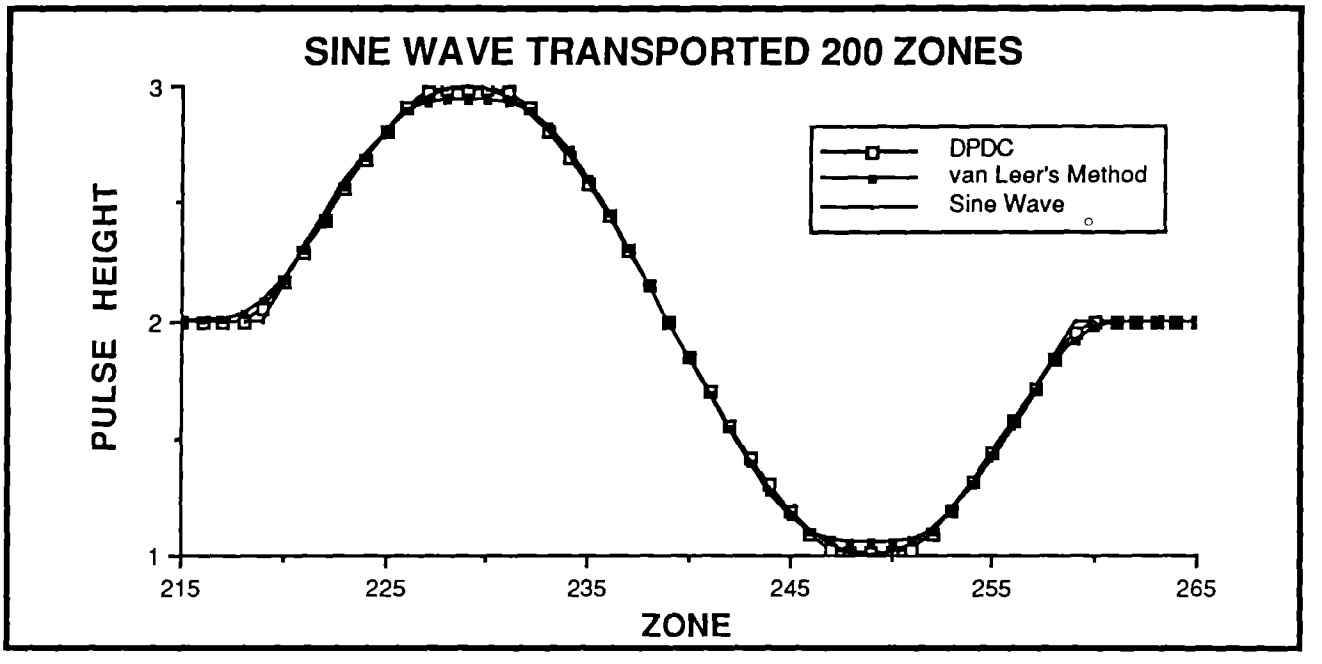


Figure 4. A sinusoidal wave is advected with a constant velocity for 200 zones. The DPDC calculation is compared with a Van Leer scheme, and with the original profile.

ACKNOWLEDGMENTS

Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

REFERENCES

1. R. B. Demuth, L. G. Margolin, B. D. Nichols, T. F. Adams and B. W. Smith, SHALE: A Computer Program for Solid Dynamics," Los Alamos National Laboratory Report LA-10236, May, 1985.

2. L. D. Cloutman, "A Convective Flux Limiter for Non-Lagrangian Computational Fluid Dynamics," **J. Comp. Phys.** 73, 349 (1987).

3. P. K. Sweby, "High Resolution Schemes Using Flux Limiters for Hyperbolic Conservation Laws," **SIAM J. Num. Anal.** 21, 995 (1984).

4. P. K. Smolarkiewicz, "A Simple Positive Definite Advection Scheme with Small Implicit Diffusion," **Mon. Weather Rev.** 111, 479 (1983).

5. P. K. Smolarkiewicz and T. L. Clark, "The Multidimensional Positive Definite Advection Transport Algorithm," **J. Comp. Phys.** 67, 396 (1986).